Misconceptions in Near-Infrared Calibration Development: Evaluating Crop-Specific vs. Mixed-Crop Calibrations

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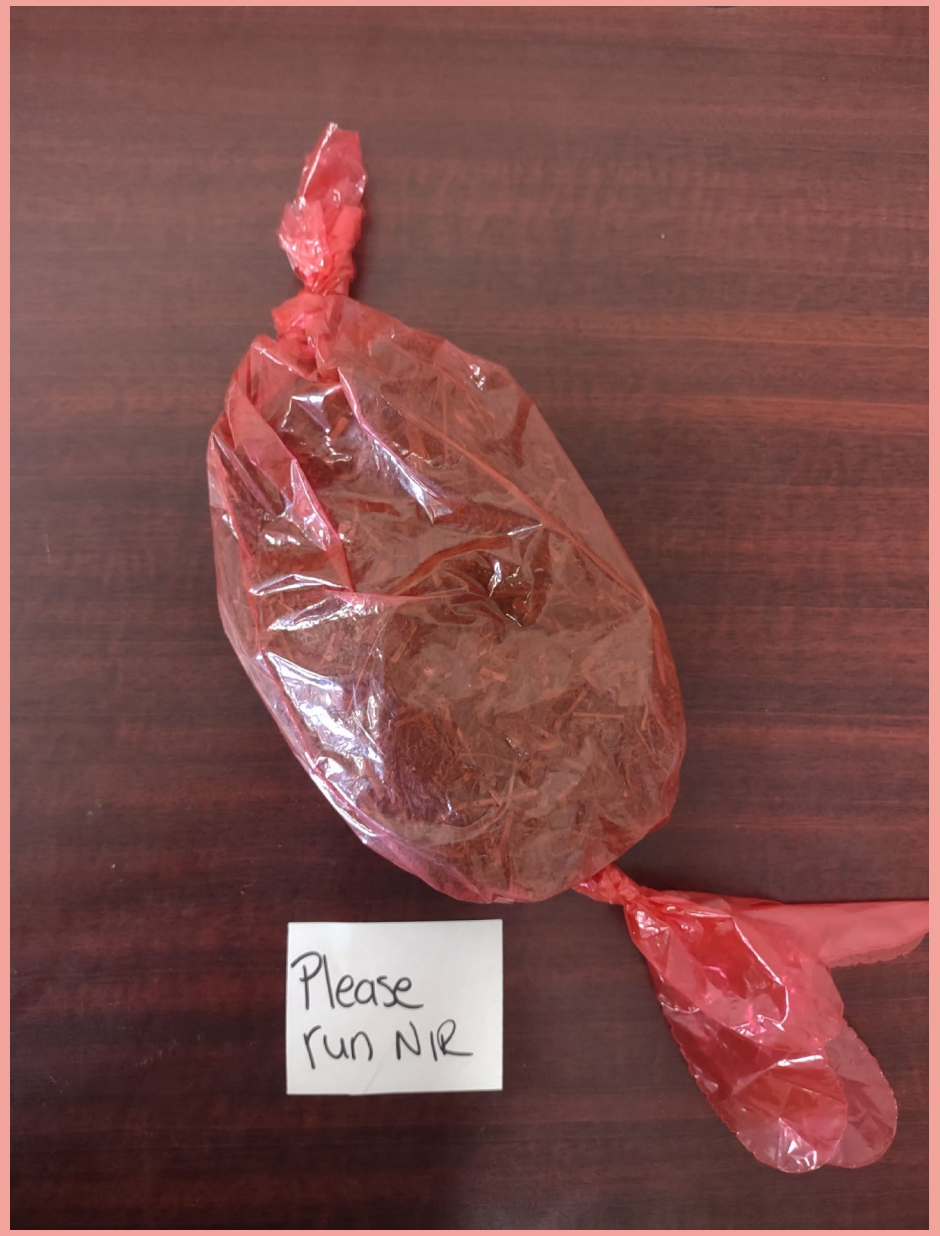
Background

- Most studies support crop-specific near-infrared (NIR) calibrations for increased accuracy
  (Yang, 2024; Andueza et al., 2011; Berzaghi et al., 2000)

- Some commercial laboratories use mixed-crop NIR calibrations
  (Kern-Lunbery and Husmoen, 2023)

- Differences in sample metadata and operational needs contribute to this disconnect



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Background: NIR Calibration Development

Robust

- Wide range of residual DM (ex. 86 – 100%)
- May include multiple crops, regions, and/or hybrids
- Can handle variability across different conditions

Accurate

- Narrow range of residual DM (ex. 92 – 100%)
- Calibrations may be specific for crop, region, and/or hybrid
- Highly defined for particular conditions

Objective

- Bridge gaps in understanding between research and industry in NIR calibration development for commercial use
  - Compare sorghum/sudan silage predicted using mixed-crop (small grain silage: barley, wheat, oats, rye, sorghum/sudan, etc, and their mixtures) vs. crop-specific NIR calibrations
  - Compare ensiled alfalfa predicted using mixed-crop (mixed alfalfa/legume: alfalfa, grass, clover, etc, and their mixtures) vs. crop-specific NIR calibrations

Materials and methods

- Sample information
  - 312 ensiled sorghum/sudan
  - 842 ensiled alfalfa
  - 2021 – 2023 crop years (May 2021 – April 2024)
  - Source: Dairyland Laboratories, Inc

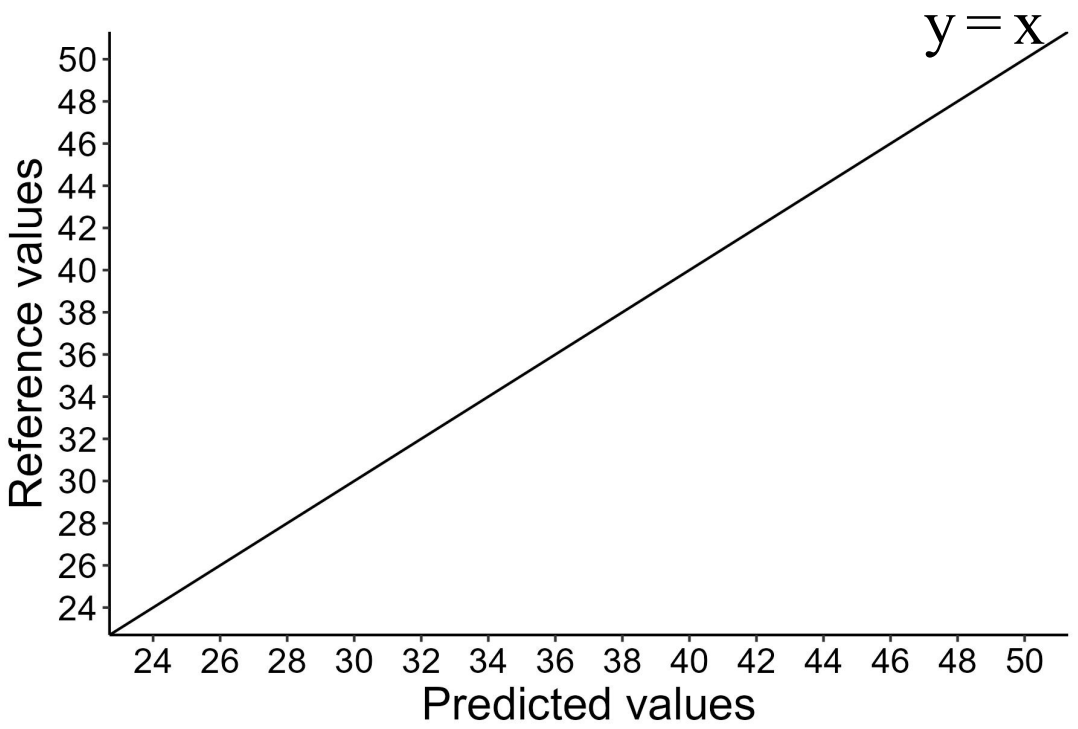
- Subset for analysis
  - 50 sorghum/sudan and 300 alfalfa samples
  - Selected to evenly represent normal ranges for CP, ADF, aNDFom

Materials and methods

- Analysis
  - Chemistry (AOAC, 2023)
    - CP, ADF, aNDFom
  - Near-infrared reflective spectroscopy (NIR)
    - Spectra collected every 2 nm over 1100–2500 nm wavelength range
      - Sorghum/sudan: Predicted using sorghum/sudan-specific and mixed small grain silage calibrations (barley, wheat, oats, rye, sorghum/sudan, etc, and their mixtures)
      - Alfalfa: Predicted using alfalfa-specific and mixed legume/grass calibrations (alfalfa, grass, clover, etc, and their mixtures)

Materials and methods: Statistics

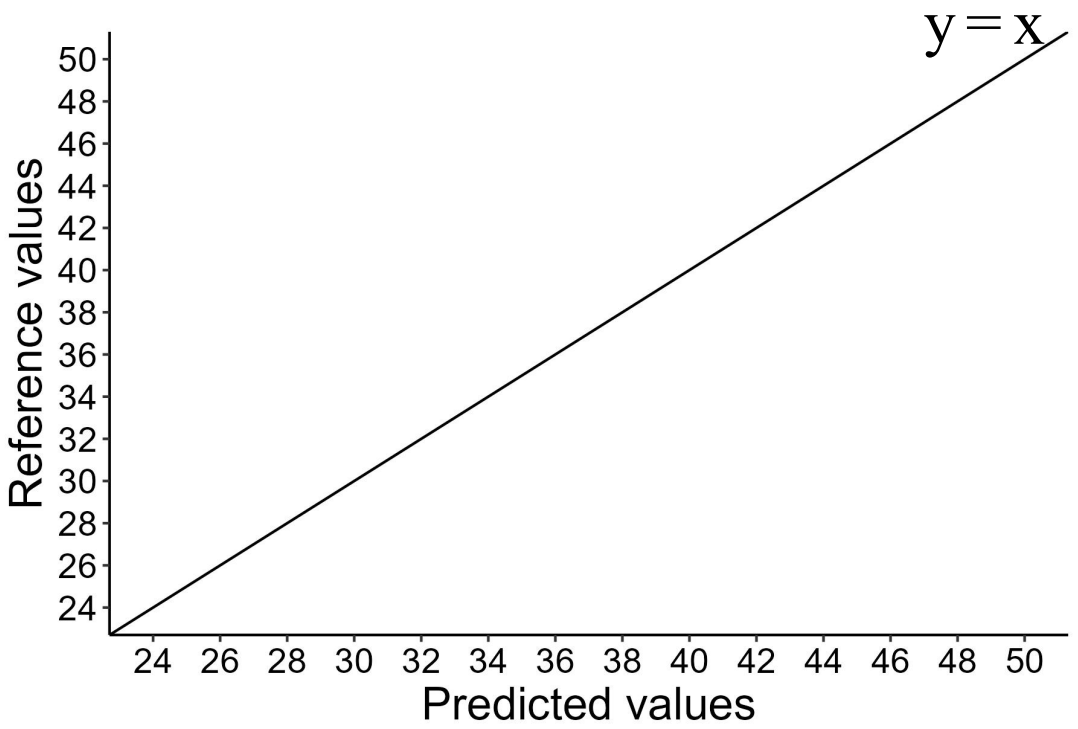
- Statistics
  - Slope = $\frac{\Delta \text{Chemistry}}{\Delta \text{NIR}}$
  - Bias = $\text{Mean}_{\text{NIR}} - \text{Mean}_{\text{Chemistry}}$
  - Standard error of prediction (SEP)
  - R^2



Materials and methods: Statistics

- Statistics
  - Slope evaluation
    - Tested whether slopes differed
      - From 1
      - Between mixed-crop vs. crop specific calibrations
        - Sorghum/sudan-specific vs. mixed small grain silages
        - Alfalfa-specific vs. mixed grass/legume

lstrends() from the 'emmeans' package in R (Lenth, 2022)

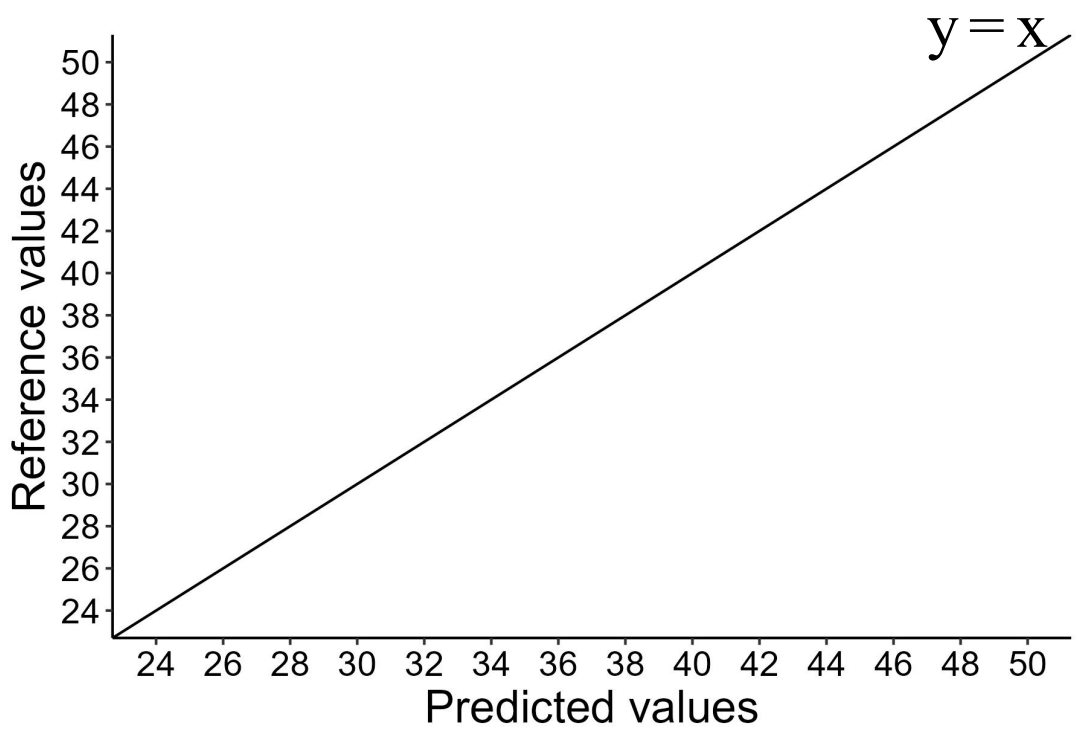


$$\text{Slope} = \frac{\Delta \text{Chemistry}}{\Delta \text{NIR}}$$

Materials and methods: Statistics

- Statistics
  - Bias evaluation
    - Tested whether the bias differed
      - From 0
      - Between mixed-crop vs. crop specific calibrations
        - Sorghum-specific vs. mixed small grain silages
        - Alfalfa-specific vs. mixed grass/legume

contrast() from the 'emmeans' package in R (Lenth, 2022)



$$\text{Bias} = \text{Mean}_{\text{NIR}} - \text{Mean}_{\text{Chemistry}}$$

Materials and methods: Statistics

- Statistics
  - SEP compared using F-Test (Snedcor & Cochran, 1989)
    - Crop-specific vs. mixed-crop calibrations
      - Sorghum/sudan-specific vs. mixed small grain silages
      - Alfalfa-specific vs. mixed grass/legume

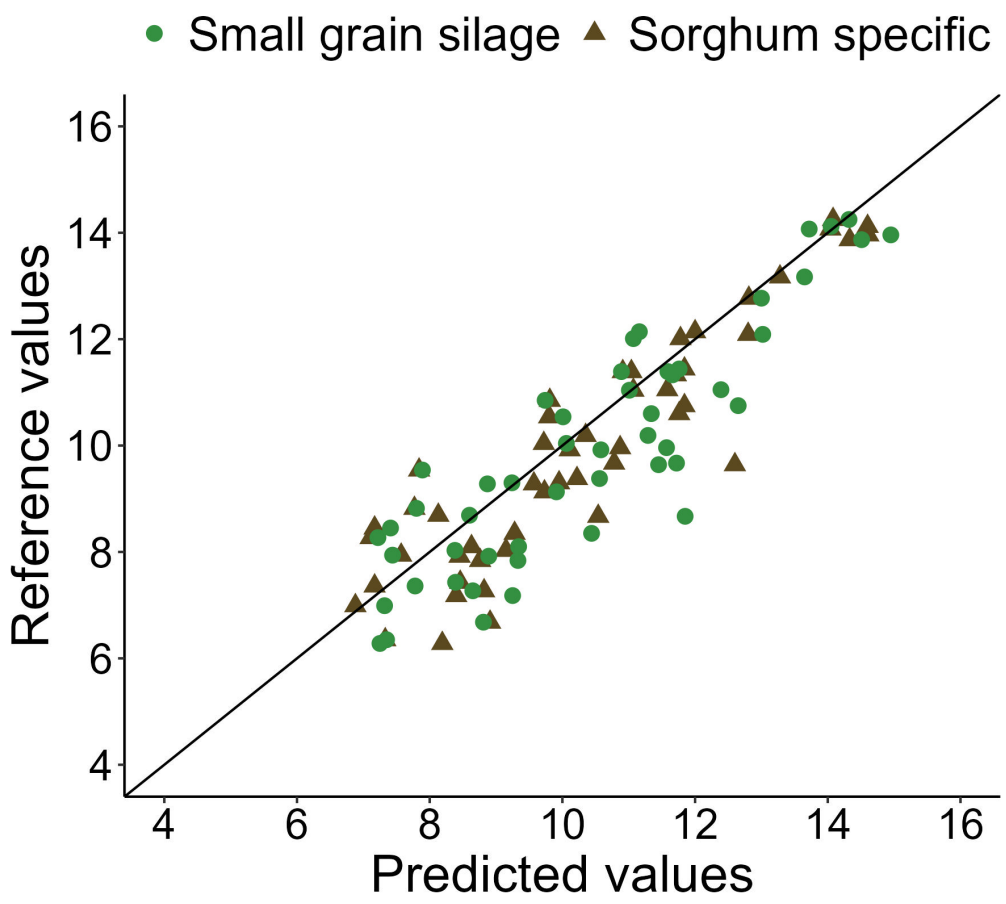
$$\text{F value} = \frac{SEP_{Lg}{}^2}{SEP_S{}^2}$$

Lg = larger SEP, S = smaller SEP of the pair

Results: Sorghum/sudan silage CP

	Mixed -SGS	SS	SE	P-value
SEP	1.15	0.98	-	0.14
Slope	0.90	0.93	0.07	0.71
Bias	-0.51*	-0.37*	0.16	0.38
R^2	0.79	0.83	-	-

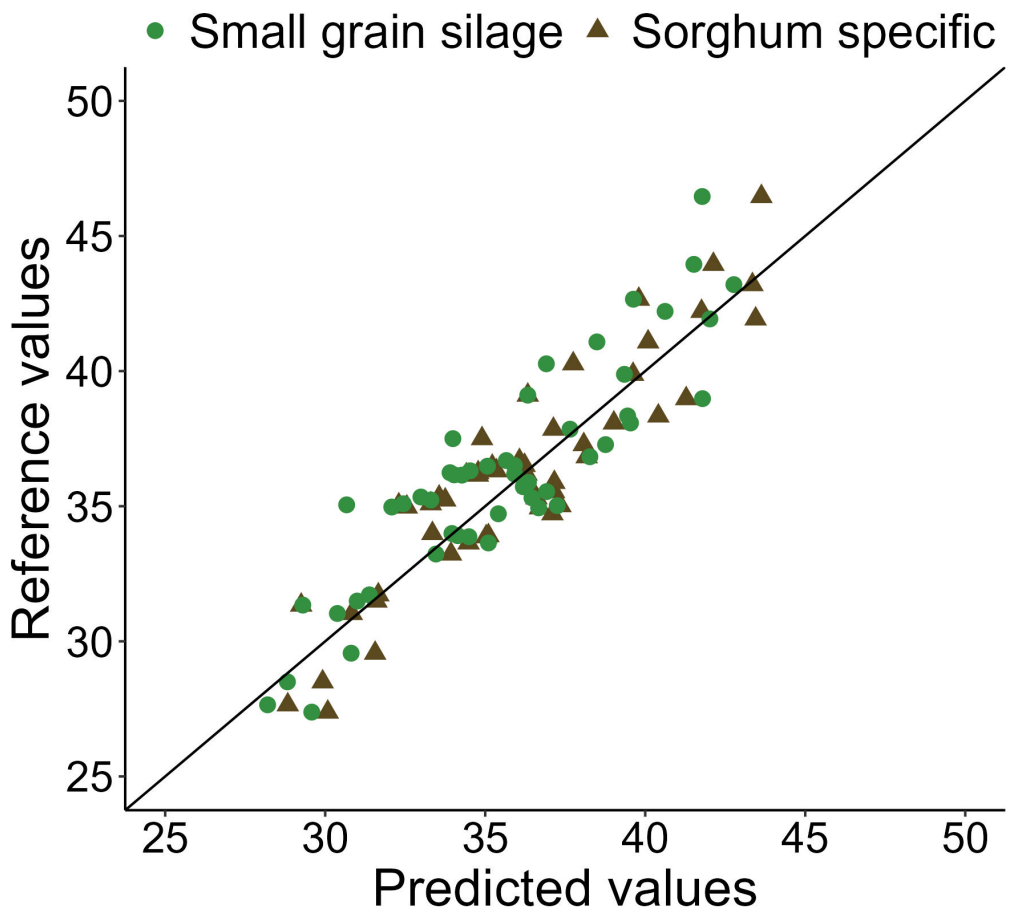
*Bias < 0, p < 0.05



Results: Sorghum/sudan silage ADF

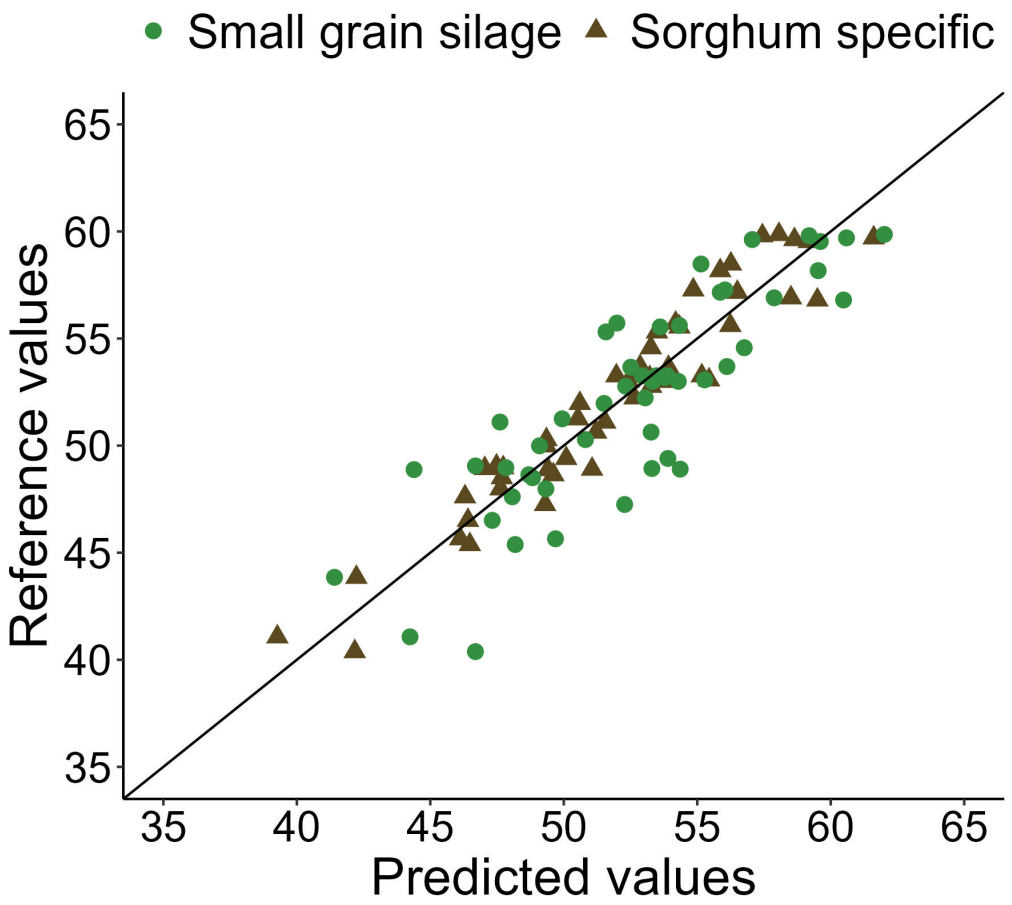
	Mixed -SGS	SS	SE	P-value
SEP	1.92	1.63	-	0.13
Slope	0.97	0.99	0.08	0.79
Bias	0.62^{+}	0.14	0.2	0.09
R^2	0.79	0.83	-	-

$^{+}$Bias tended to be > 0, $p = 0.06$



Results: Sorghum/sudan silage aNDFom

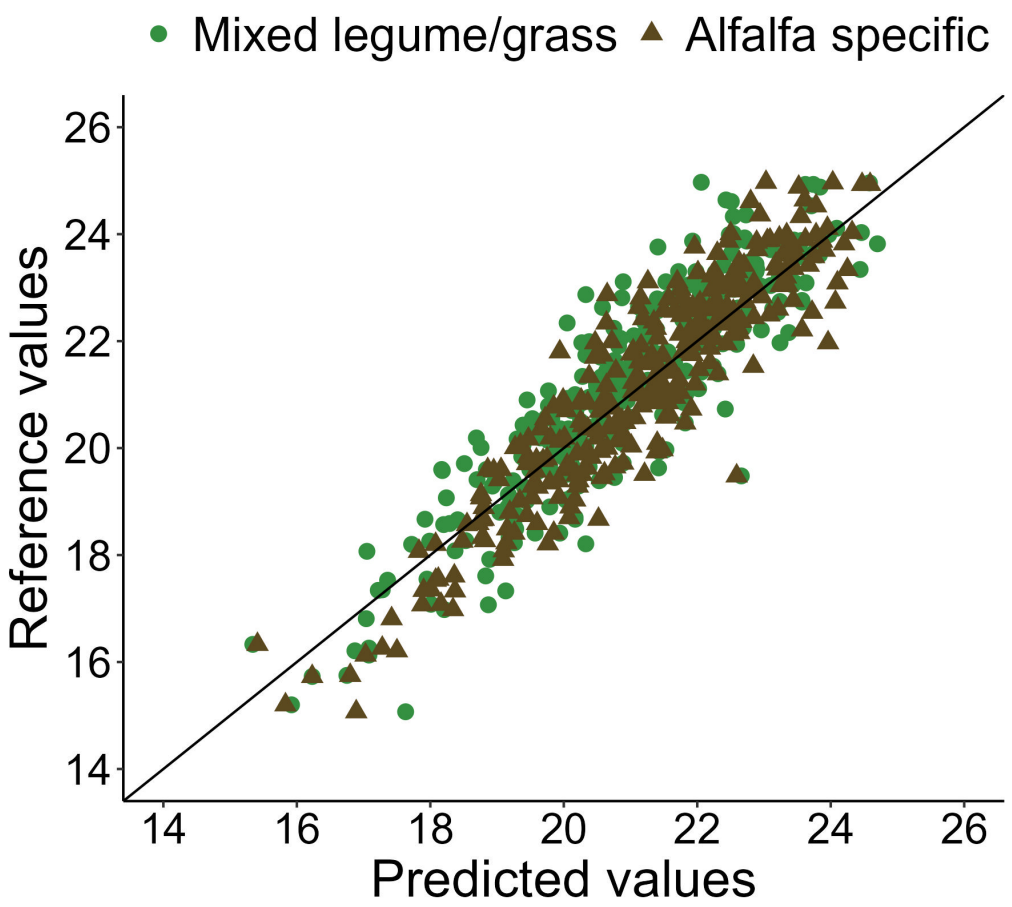
	Mixed -SGS	SS	SE	P-value
SEP	2.54	1.40	-	< 0.001
Slope	0.91	0.97	0.07	0.39
Bias	-0.47	0.25	0.24	< 0.05
R^2	0.73	0.92	-	-



Results: Ensiled alfalfa CP

	Mixed LEG/GR	Alfalfa	SE	P-value
SEP	0.93	0.80	-	<0.01
Slope	1.04	1.09*	0.03	0.11
Bias	0.22*	-0.01	0.04	< 0.001
R^2	0.80	0.85	-	-

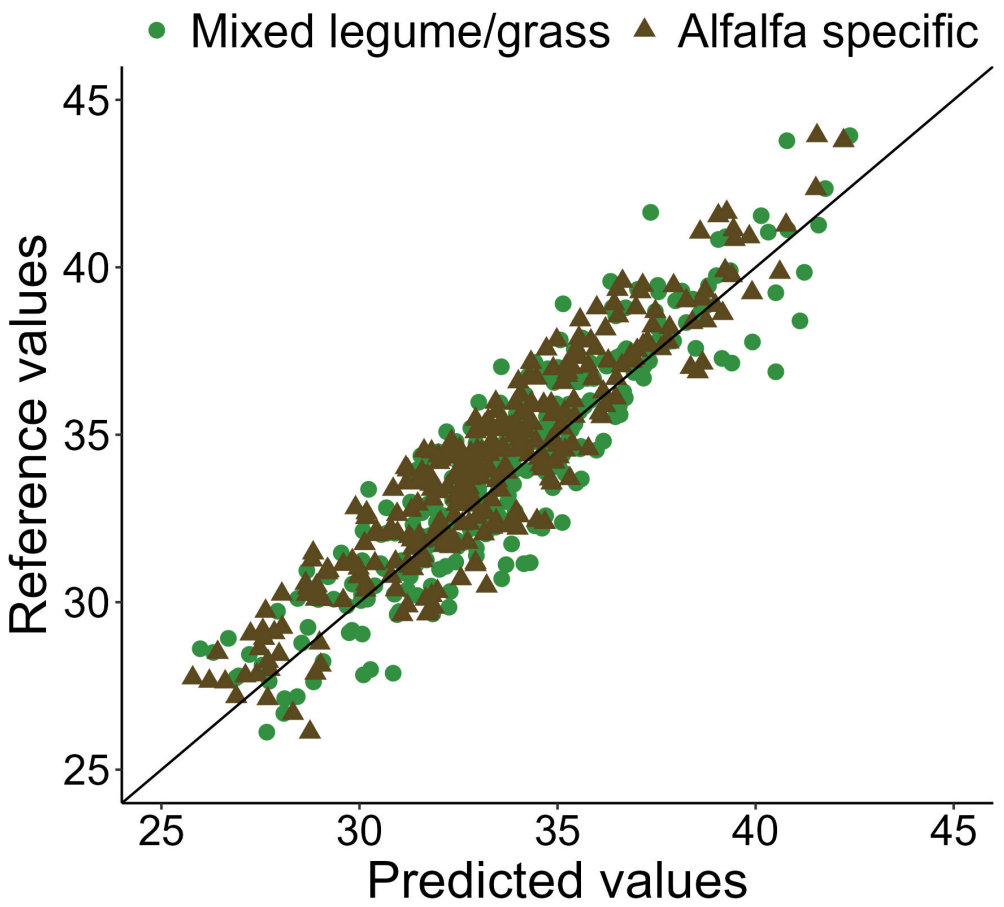
*Slope was > 1, Bias was > 0, p < 0.05



Results: Ensiled alfalfa ADF

	Mixed LEG/GR	Alfalfa	SE	P-value
SEP	1.45	1.47	-	0.38
Slope	0.97	0.98	0.03	0.87
Bias	0.36*	0.77*	0.06	< 0.001
R^2	0.82	0.86	-	-

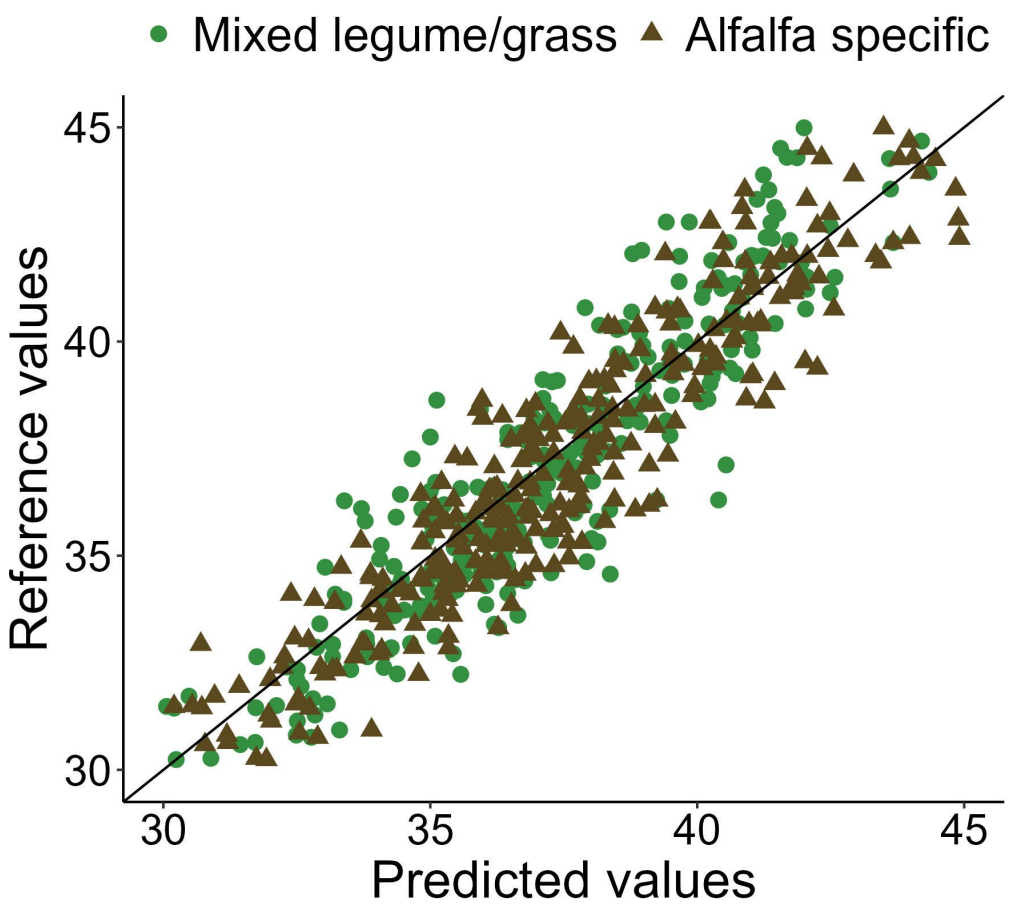
*Bias was > 0, p < 0.05



Results: Ensiled alfalfa aNDFom

	Mixed LEG/GR	Alfalfa	SE	P-value
SEP	1.41	1.29	-	0.06
Slope	1.02	0.98	0.03	0.21
Bias	-0.13	-0.27*	0.06	0.10
R^2	0.83	0.86	-	-

*Bias was < 0, $p < 0.05$

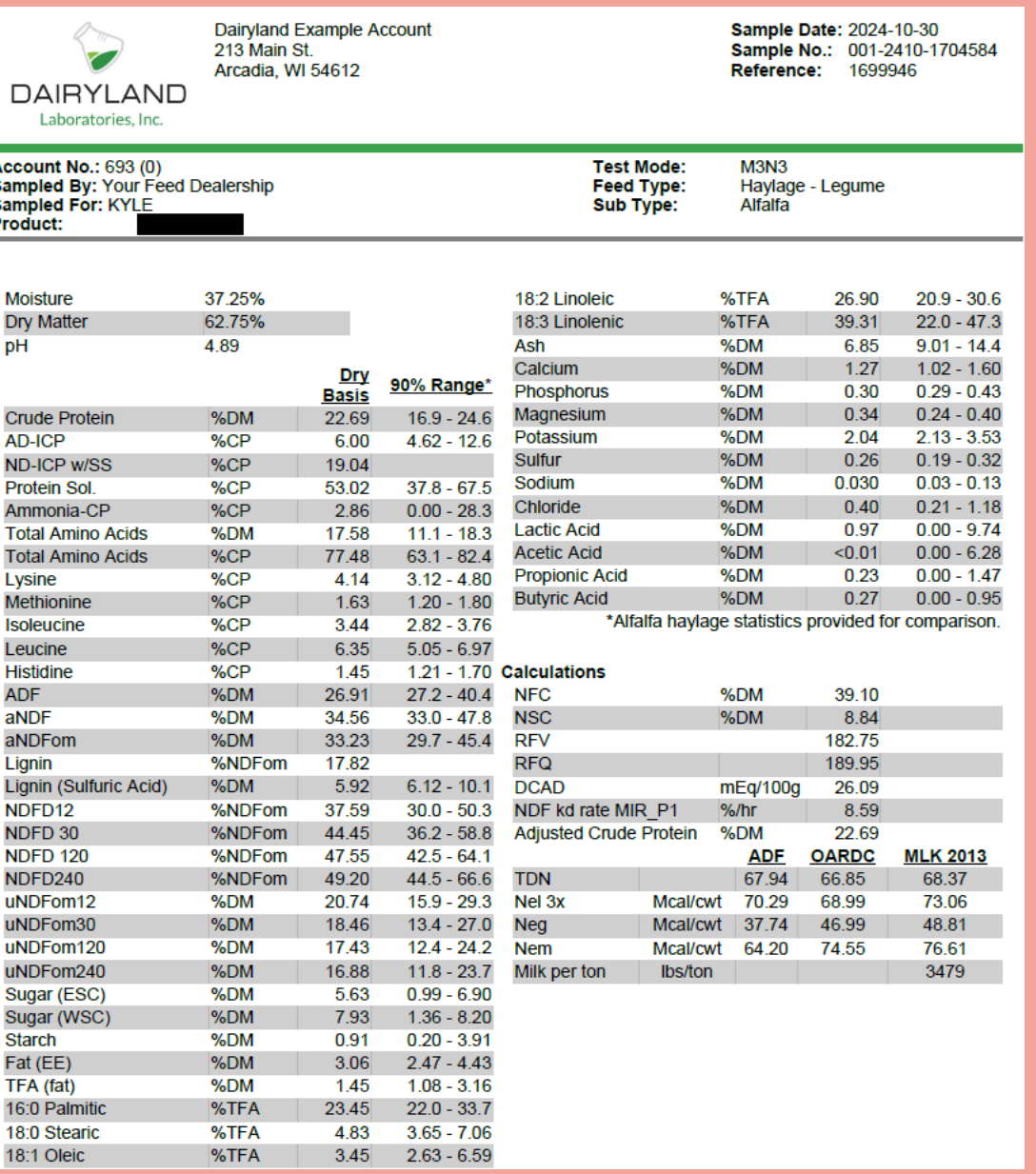


Summary

- Commercial calibration decisions may diverge from theoretical ideals
  - No single calibration strategy is ideal for all scenarios
- Broader calibrations prioritize applicability across diverse samples, at the expense of accuracy compared to more narrowly focused models (Shenk and Westerhaus, 1993)
- Evaluation metrics must be interpreted in context
  - Low R^2, significant deviations of slope from 1 or biases from 0 are not always problematic

Summary

- Feed reports include linked parameters, ex:
  - CP, Protein solubility
  - aNDFom, NDFD12, NDFD30, NDFD120, NDFD240
  - WSC, ESC



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Dairyland Example Account
213 Main St.
Arcadia, WI 54612

Sample Date: 2024-10-30
Sample No.: 001-2410-1704584
Reference: 1699946

Account No.: 693 (0)
Sampled By: Your Feed Dealership
Sampled For: KYLE
Product: [redacted]

Test Mode: M3N3
Feed Type: Haylage - Legume
Sub Type: Alfalfa

Moisture	37.25%		
Dry Matter	62.75%		
pH	4.89		

		Dry Basis	90% Range*
Crude Protein	%DM	22.69	16.9 - 24.6
AD-ICP	%CP	6.00	4.62 - 12.6
ND-ICP w/SS	%CP	19.04	
Protein Sol.	%CP	53.02	37.8 - 67.5
Ammonia-CP	%CP	2.86	0.00 - 28.3
Total Amino Acids	%DM	17.58	11.1 - 18.3
Total Amino Acids	%CP	77.48	63.1 - 82.4
Lysine	%CP	4.14	3.12 - 4.80
Methionine	%CP	1.63	1.20 - 1.80
Isoleucine	%CP	3.44	2.82 - 3.76
Leucine	%CP	6.35	5.05 - 6.97
Histidine	%CP	1.45	1.21 - 1.70
ADF	%DM	26.91	27.2 - 40.4
aNDF	%DM	34.56	33.0 - 47.8
aNDFom	%DM	33.23	29.7 - 45.4
Lignin	%NDFom	17.82	
Lignin (Sulfuric Acid)	%DM	5.92	6.12 - 10.1
NDFD12	%NDFom	37.59	30.0 - 50.3
NDFD 30	%NDFom	44.45	36.2 - 58.8
NDFD 120	%NDFom	47.55	42.5 - 64.1
NDFD240	%NDFom	49.20	44.5 - 66.6
uNDFom12	%DM	20.74	15.9 - 29.3
uNDFom30	%DM	18.46	13.4 - 27.0
uNDFom120	%DM	17.43	12.4 - 24.2
uNDFom240	%DM	16.88	11.8 - 23.7
Sugar (ESC)	%DM	5.63	0.99 - 6.90
Sugar (WSC)	%DM	7.93	1.36 - 8.20
Starch	%DM	0.91	0.20 - 3.91
Fat (EE)	%DM	3.06	2.47 - 4.43
TFA (fat)	%DM	1.45	1.08 - 3.16
16:0 Palmitic	%TFA	23.45	22.0 - 33.7
18:0 Stearic	%TFA	4.83	3.65 - 7.06
18:1 Oleic	%TFA	3.45	2.63 - 6.59
18:2 Linoleic	%TFA	26.90	20.9 - 30.6
18:3 Linolenic	%TFA	39.31	22.0 - 47.3
Ash	%DM	6.85	9.01 - 14.4
Calcium	%DM	1.27	1.02 - 1.60
Phosphorus	%DM	0.30	0.29 - 0.43
Magnesium	%DM	0.34	0.24 - 0.40
Potassium	%DM	2.04	2.13 - 3.53
Sulfur	%DM	0.26	0.19 - 0.32
Sodium	%DM	0.030	0.03 - 0.13
Chloride	%DM	0.40	0.21 - 1.18
Lactic Acid	%DM	0.97	0.00 - 9.74
Acetic Acid	%DM	<0.01	0.00 - 6.28
Propionic Acid	%DM	0.23	0.00 - 1.47
Butyric Acid	%DM	0.27	0.00 - 0.95

*Alfalfa haylage statistics provided for comparison.

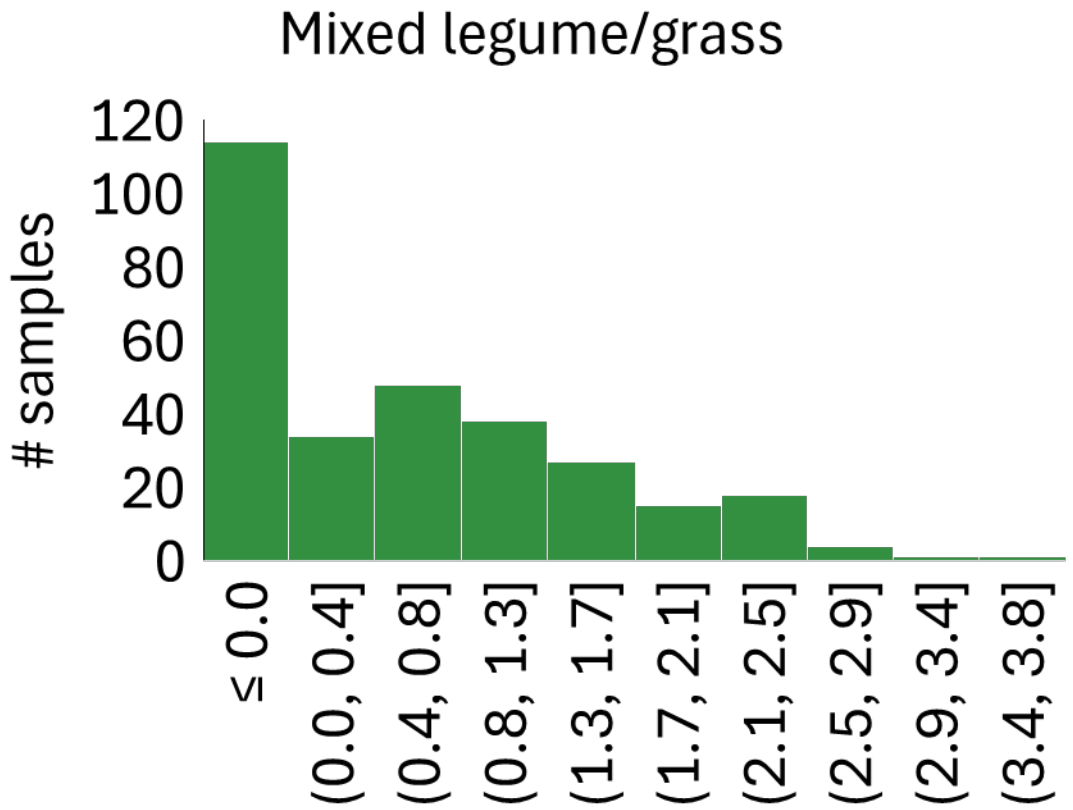
Calculations

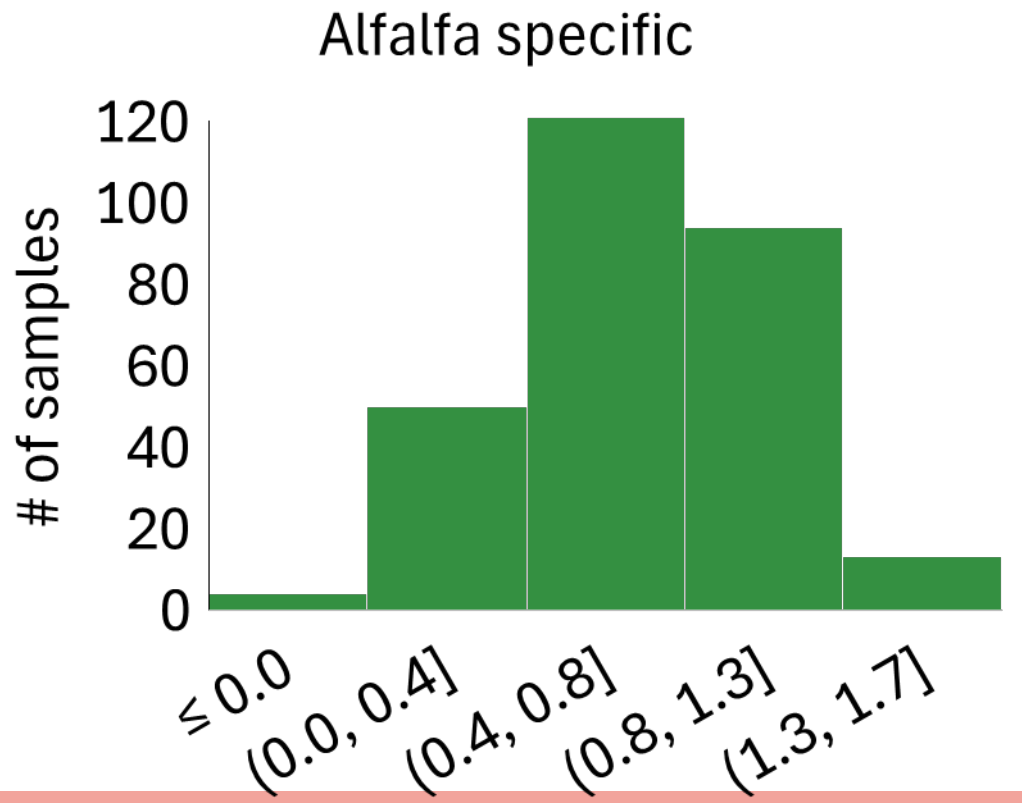
NFC	%DM	39.10
NSC	%DM	8.84
RFV		182.75
RFQ		189.95
DCAD	mEq/100g	26.09
NDF kd rate MIR_P1	%/hr	8.59
Adjusted Crude Protein	%DM	22.69

		ADF	OARDC	MLK 2013
TDN		67.94	66.85	68.37
Nel 3x	Mcal/cwt	70.29	68.99	73.06
Neg	Mcal/cwt	37.74	46.99	48.81
Nem	Mcal/cwt	64.20	74.55	76.61
Milk per ton	lbs/ton			3479

Summary

uNDFom24 – uNDFom30





DAIRYLAND Laboratories, Inc.

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